Pathway prediction for the production of high value-added chemicals

유재용, 김동인, 조아연, 윤홍석, 박진환, 이상엽*, 박선원
한국과학기술원
(leesy@kaist.ac.kr*)

Many systematic platforms have been developed to predict the metabolic pathways for efficient production of desired chemicals. Here, we developed the framework which generates pathways and suggests enzyme candidates to identify novel pathways. The systematic framework consists of two parts, route generation and prioritization process. Route generation process generates pathways based on the reaction rule sets which were based on the mechanism of existing biochemical reactions. After route generation, five prioritization factors, binding site covalence, chemical similarity, thermodynamic favorability, pathway distance and organism specificity are evaluated to estimate the feasibility of generated reaction pathways. The novel synthetic pathways for three chemicals, isobutanol, 3-hydroxypropionate (3HP) and butyryl-CoA were predicted to validate the reliability of the framework's capacity. Isobutanol producing pathway proven experimentally was reproduced and ranked at 17th among the 42,344 enzyme route candidates being within top 0.42% of the candidates. In the same manner as isobutanol, 3HP and butyryl-CoA producing pathways are validated and ranked at the second out of 4,524 enzyme route candidates and 8th out of 1,120 enzyme route candidates respectively.